

## SUPPLEMENTARY INFORMATION

# COX Inhibitory and Cytotoxic Naphthoketal-Bearing Polyketides from *Sparticola junci*

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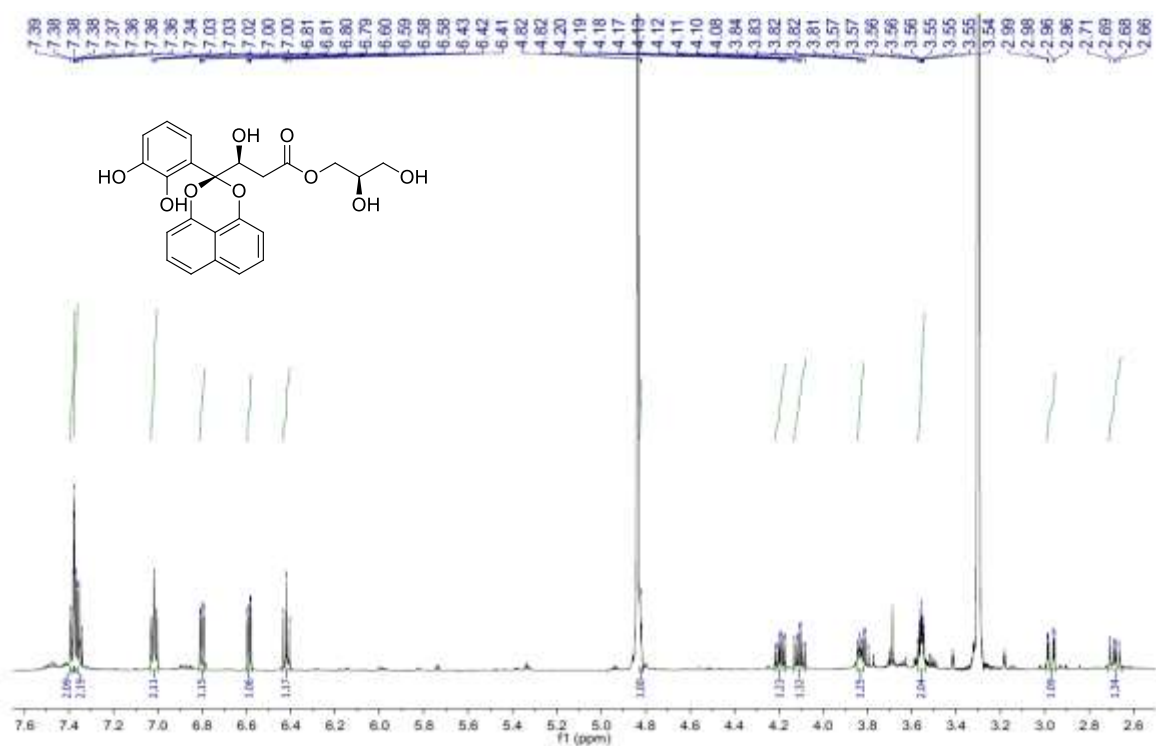
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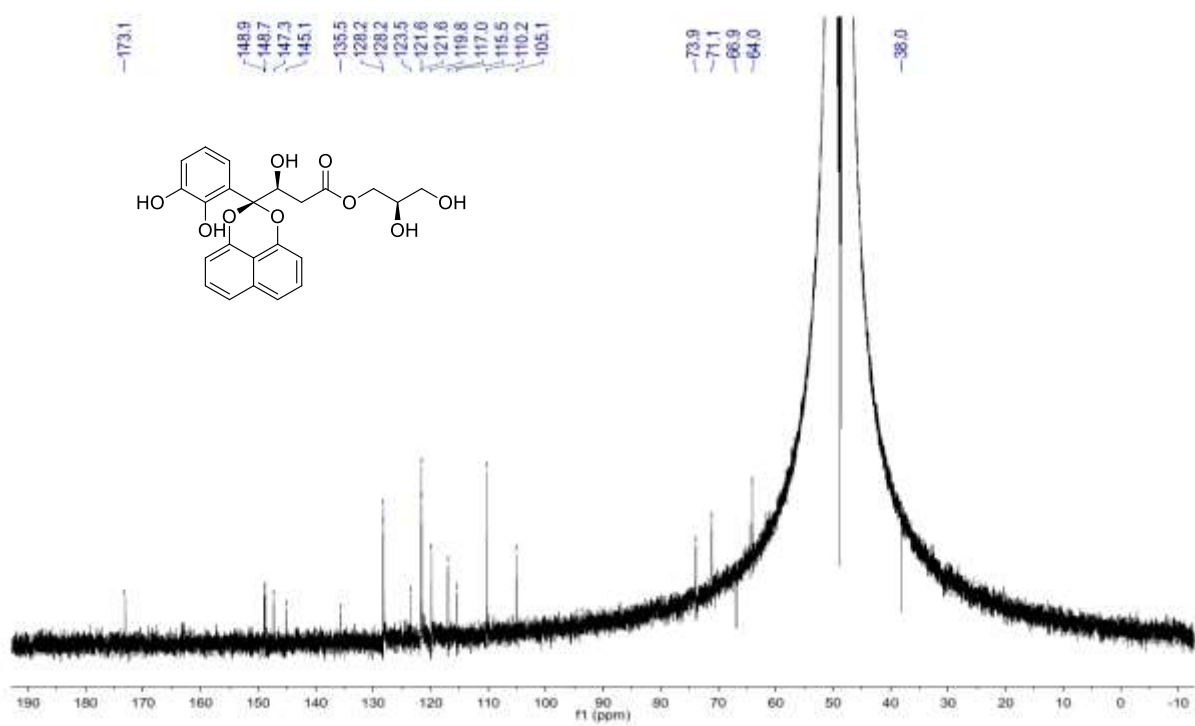
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## LIST OF SUPPORTING INFORMATION

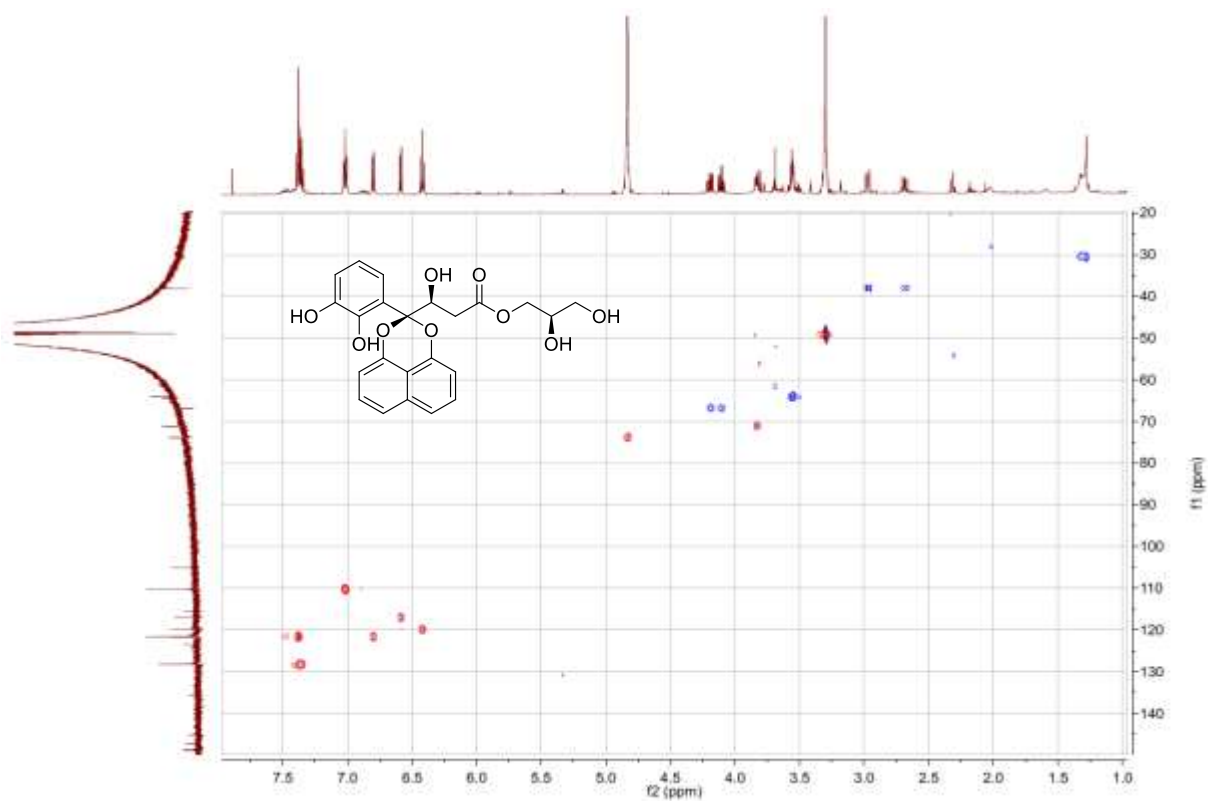
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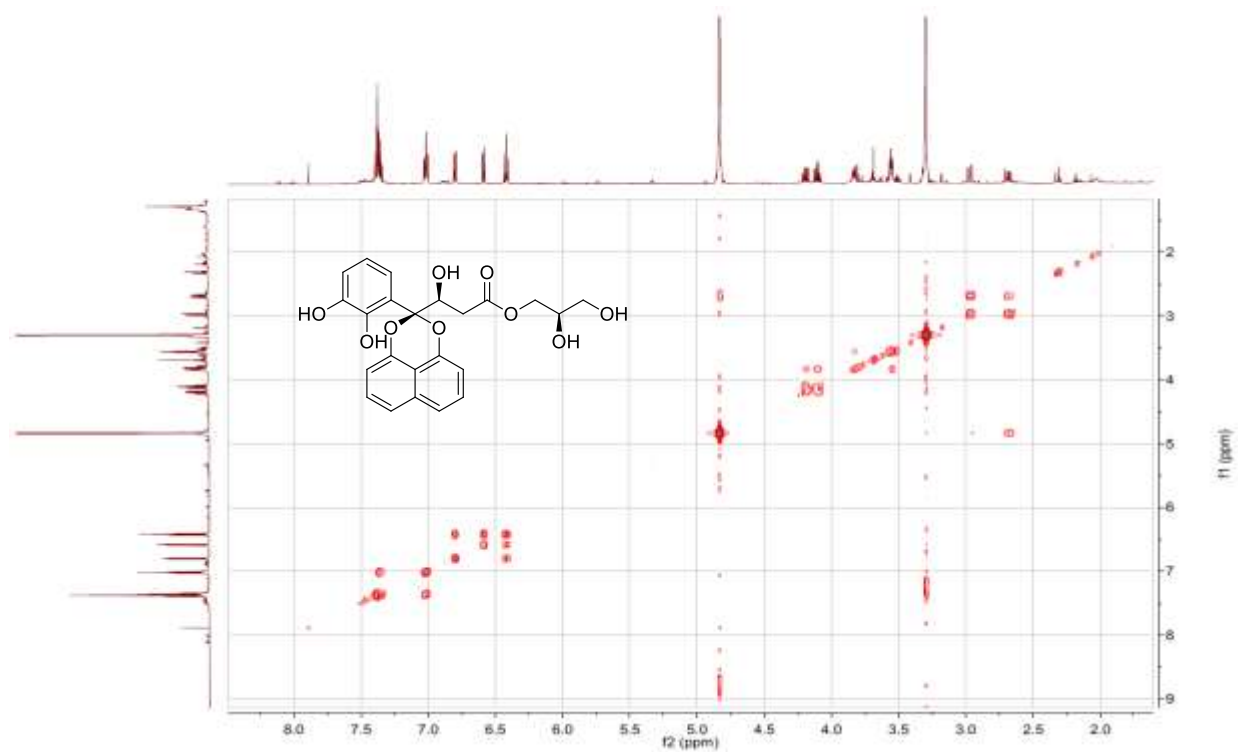
**Figure S1.** <sup>1</sup>H NMR spectrum (MeOH-*d*<sub>4</sub>, 600 MHz) of sparticatechol A (1)



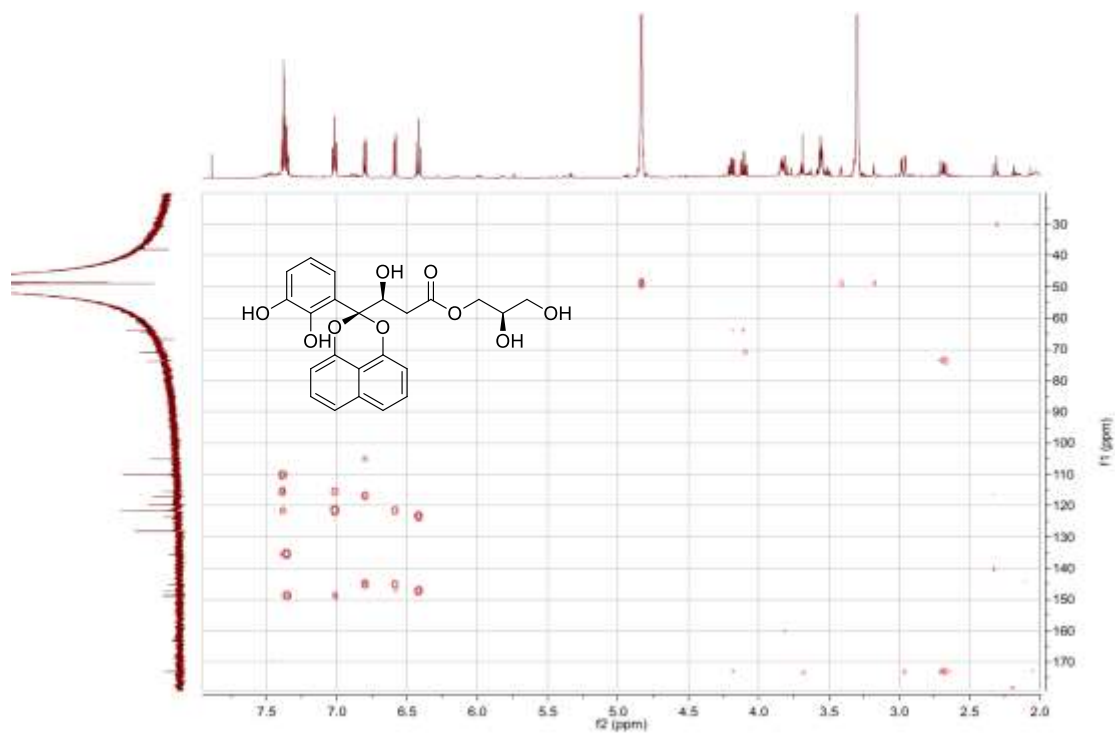
**Figure S2.** <sup>13</sup>C NMR spectrum (MeOH-*d*<sub>4</sub>, 600 MHz) of sparticatechol A (1)



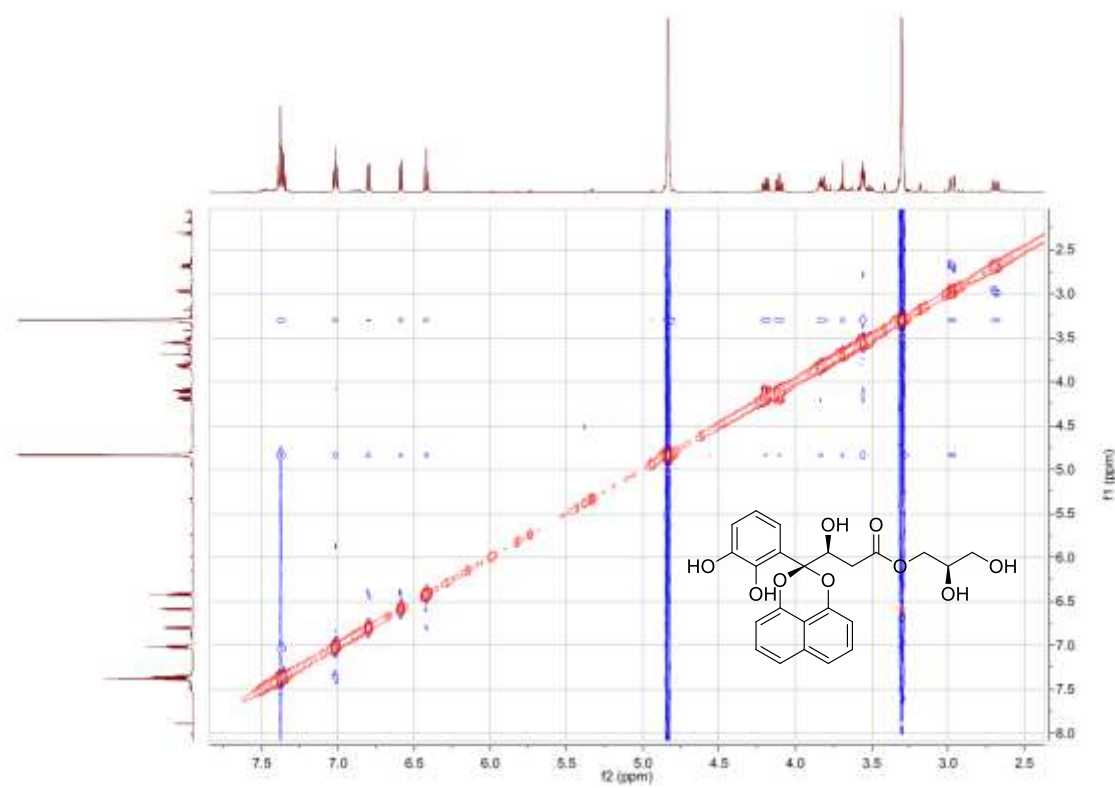
**Figure S3.** HSQC-DEPT spectrum of sparticatechol A (1)



**Figure S4.** COSY spectrum of sparticatechol A (1)



**Figure S5.** HMBC spectrum of sparticatechol A (**1**)



**Figure S6.** ROESY spectrum of sparticatechol A (**1**)

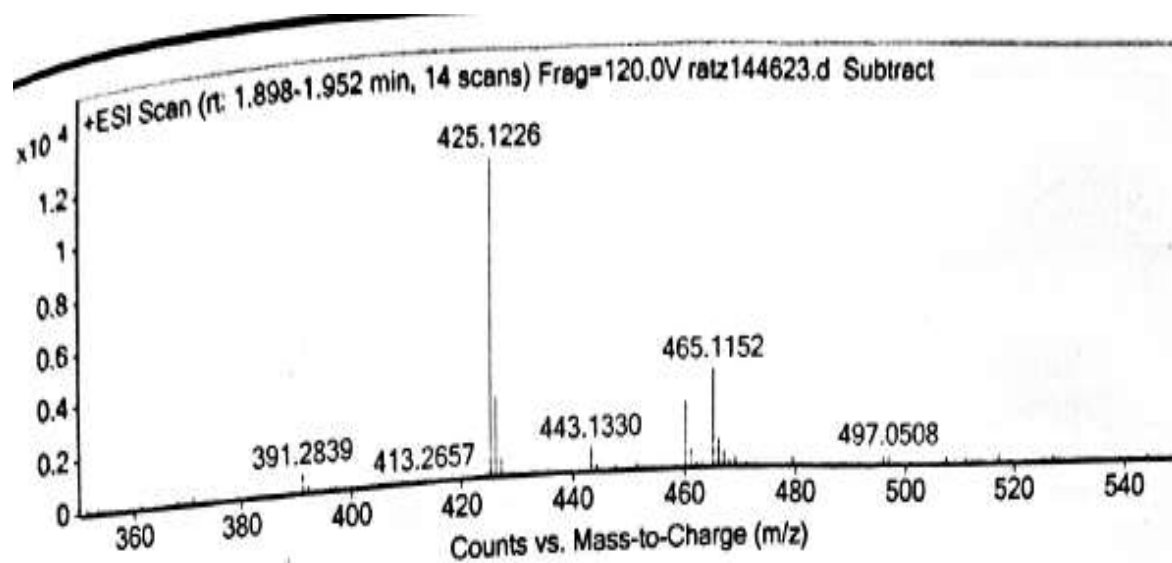
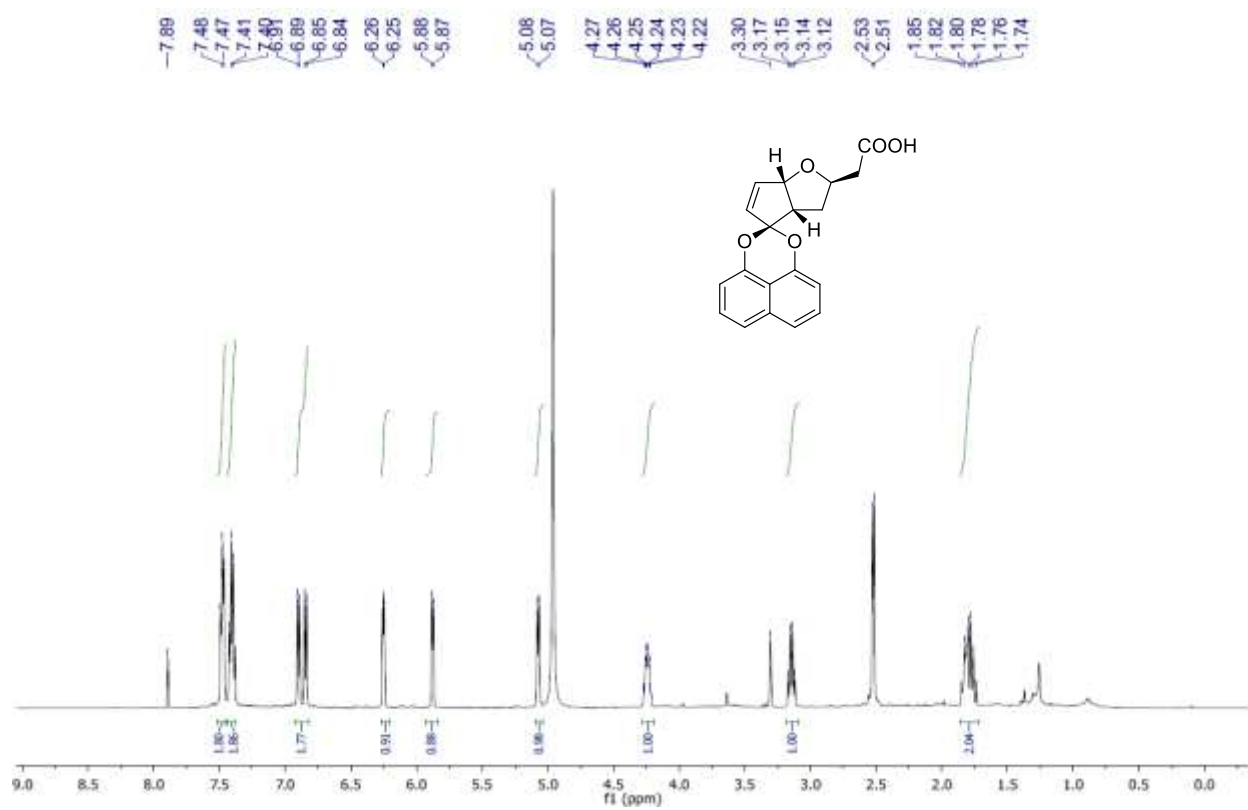
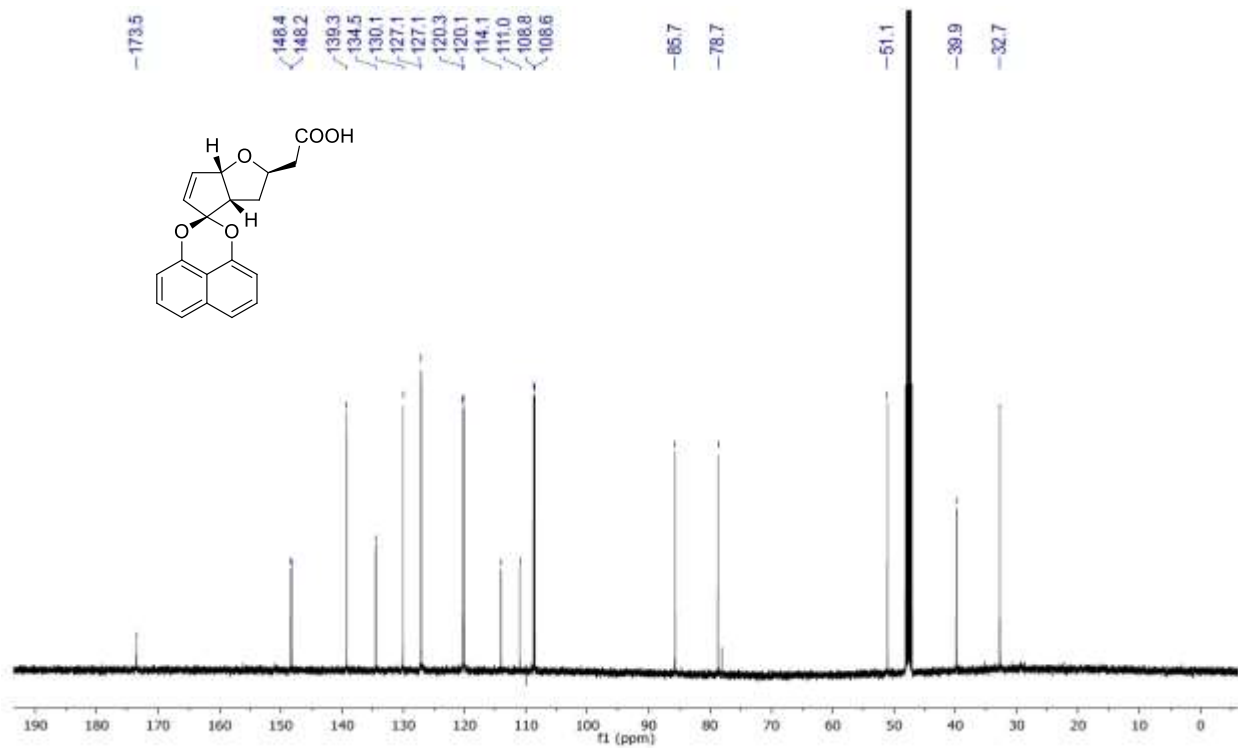


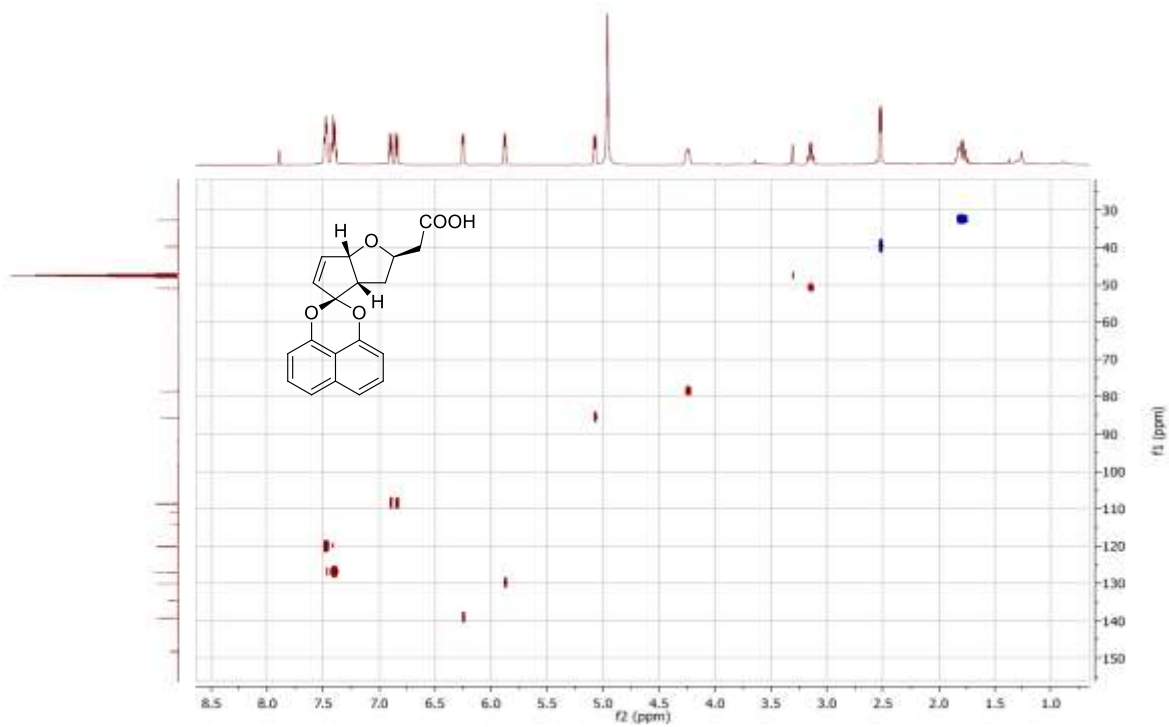
Figure S7. HR-ESIMS spectrum of sparticatechol A (1)



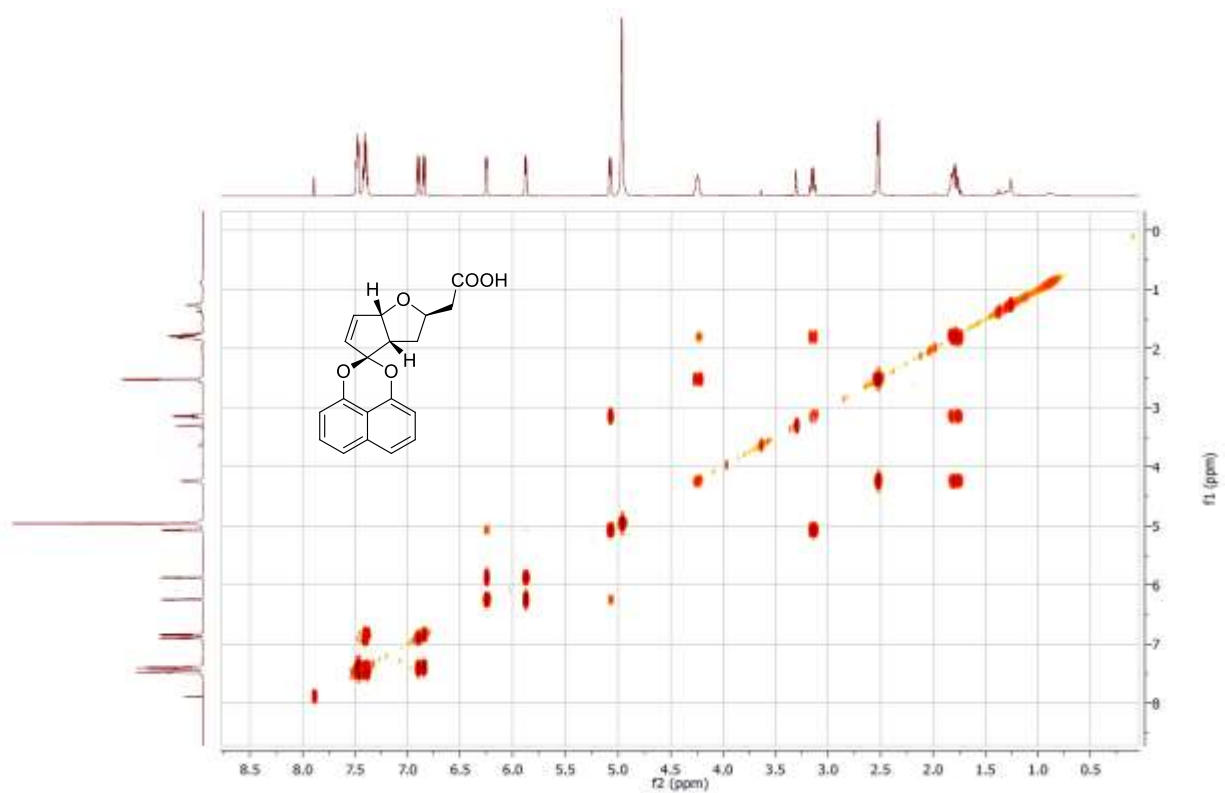
**Figure S8.** <sup>1</sup>H NMR spectrum (MeOH-*d*<sub>4</sub>, 500 MHz) of sparticolin H (2)



**Figure S9.** <sup>13</sup>C NMR spectrum (MeOH-*d*<sub>4</sub>, 125 MHz) of sparticolin H (2)

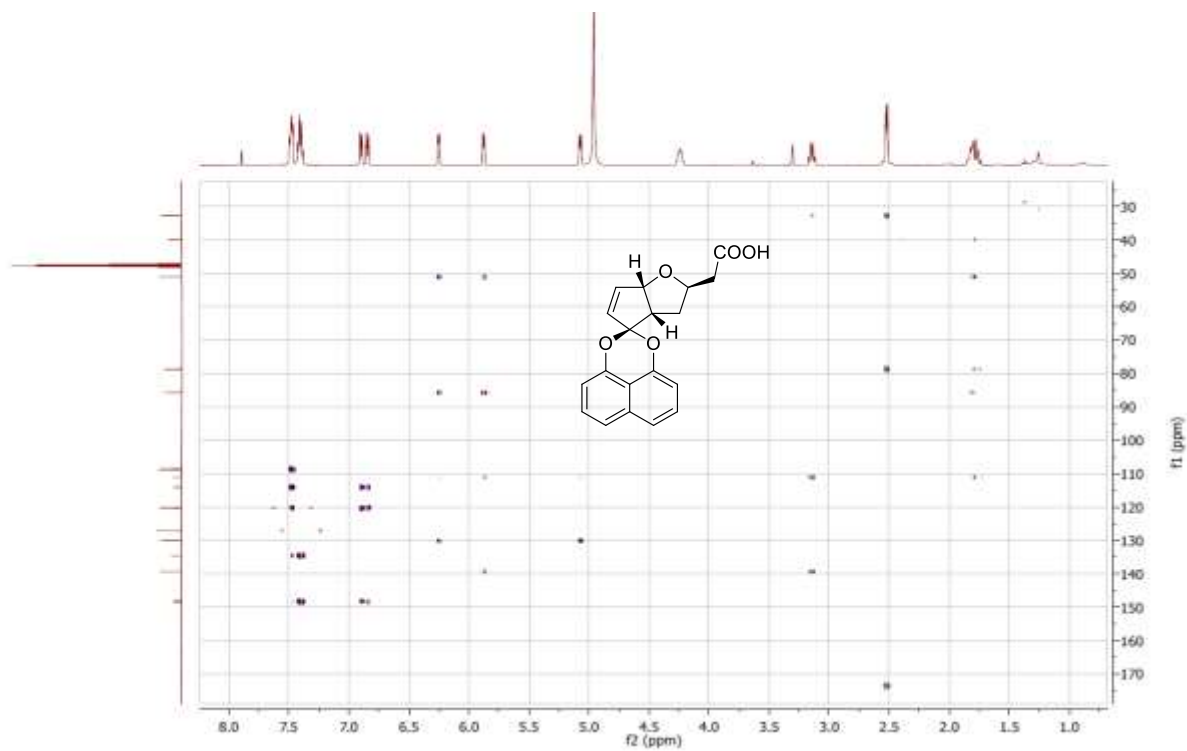


**Figure S10.** HSQC spectrum of sparticolin H (2)

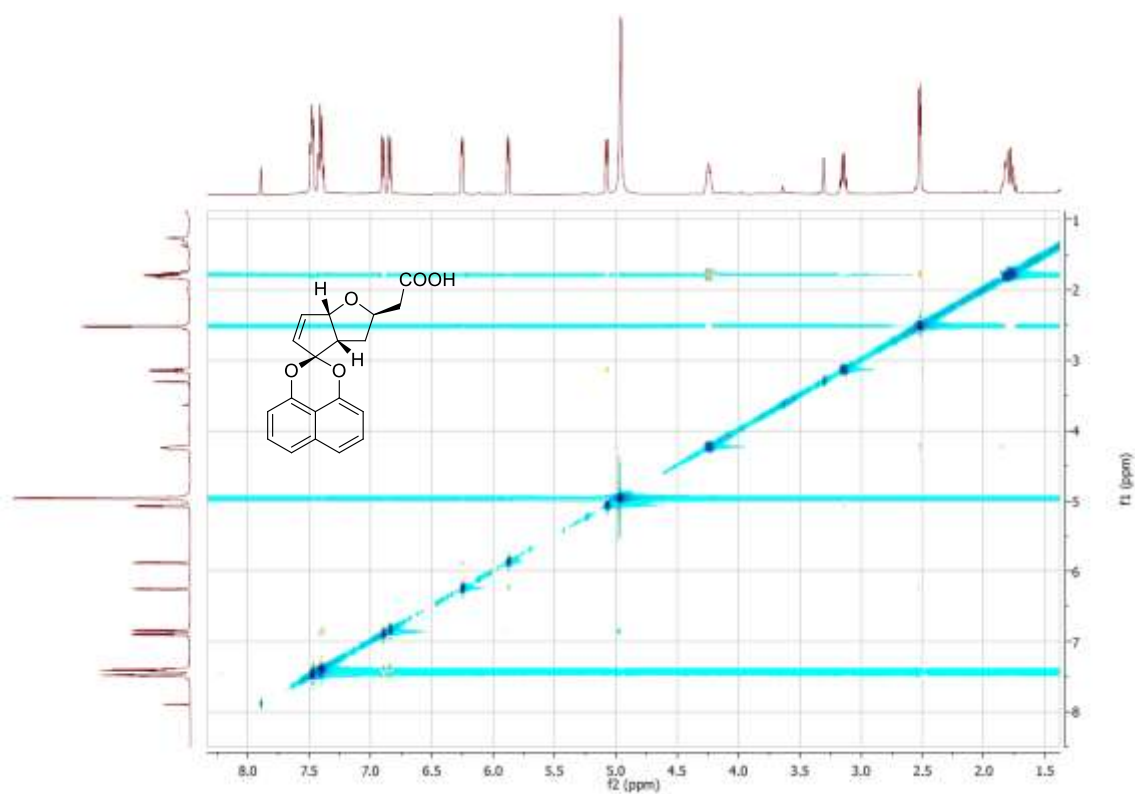


**Figure S11.** COSY spectrum of sparticolin H (2)

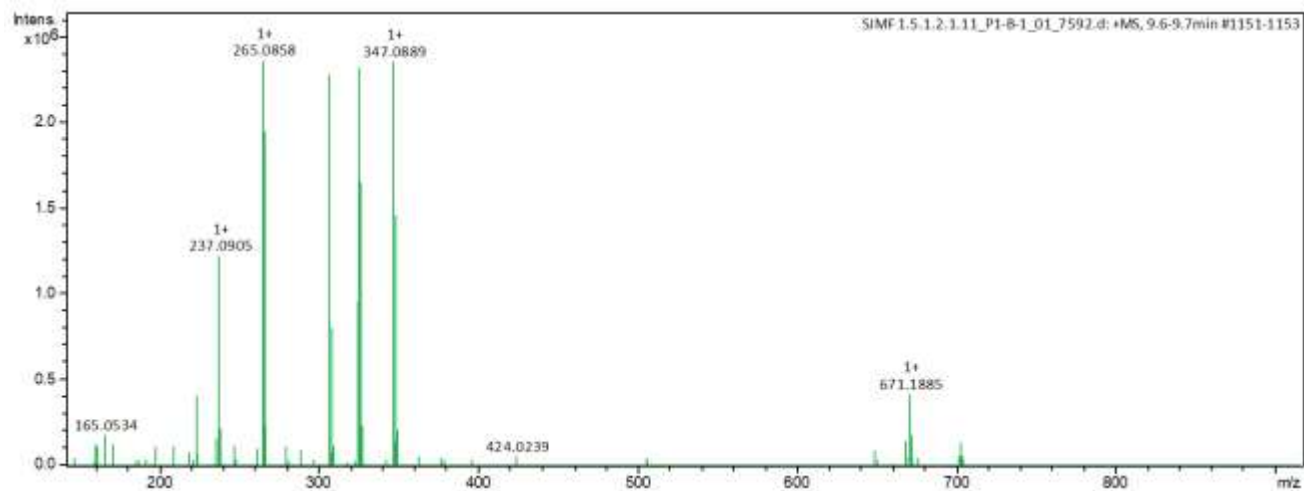




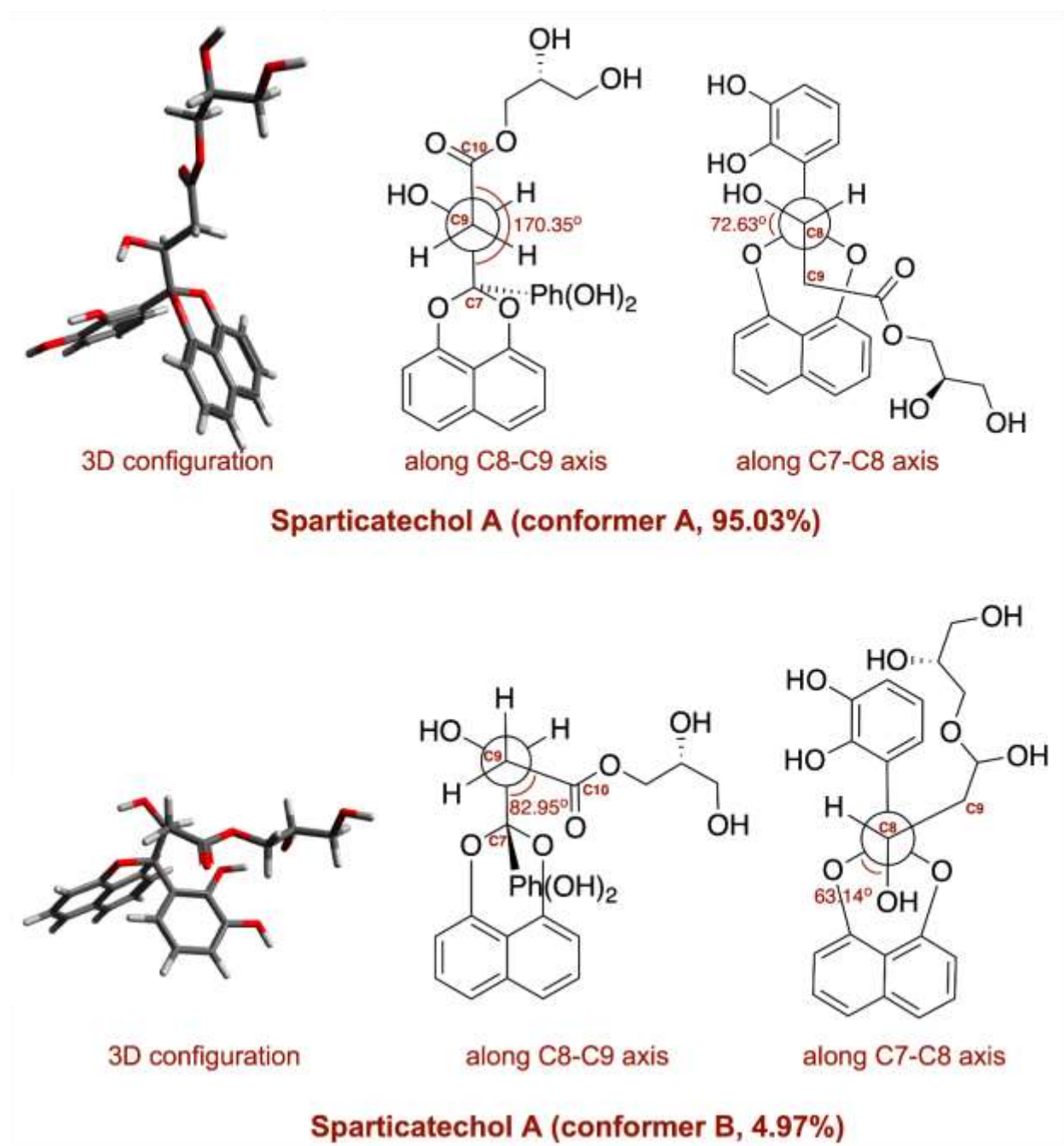
**Figure S12.** HMBC spectrum of sparticolin H (2)



**Figure S13.** NOESY spectrum of sparticolin H (2)



**Figure S14.** HR-ESIMS spectrum of sparticolin H (2)



**Figure S15.** Low energy conformers (> 1%) of (8*S*,22*R*)-**1** optimized at B3LYP/6-31G(d) (PCM/MeOH).

**Table S1.** Lipinski's rule of five for ADME analysis of compounds **1-3**.

Compound	Lipinski's Rule of Five					Drug-likeness
	Molecular weight (g/mol)	Lipophilicity (MLogP)	H-bond donor	H-bond acceptor	Rule violations	
	< 500	< 5	≤ 5	≤ 10	<2	
<b>1</b>	442.42	0.67	5	9	0	yes
<b>2</b>	324.33	2.31	1	5	0	yes
<b>3</b>	322.31	2.16	2	5	0	yes

**Table S2.** Predicted toxicity parameters of compounds **1-3**.

Compound	Mutagenicity	Tumorigenicity	Irritant Effect	Reproductive Toxicity
<b>1</b>	High Risk	None	None	None
<b>2</b>	High Risk	None	None	None
<b>3</b>	High Risk	None	None	None